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Incremental design of control system of SHARON-Anammox process for autotrophic nitrogen removal

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Abstract: With the perspective of investigating a suitable control design for autotrophic nitrogen removal, this work explores the control design for a SHARON-Anammox reactor sequence. With this aim, a full model is developed, including the pH dependency, in order to simulate the reactor and determine the optimal operating conditions. Then, the screening of controlled variables and pairing is carried out by an assessment of the effect of the disturbances based on the closed loop disturbance gain plots. Three control structures are obtained and benchmarked by their capacity to reject the disturbances before the Anammox reactor.

Keywords: Autotrophic nitrogen removal, disturbance analysis, plantwide control, modelling

1. INTRODUCTION

Complete autotrophic nitrogen removal (CANR) is especially suitable for wastewaters containing high concentrations of nitrogen and low organic carbon to nitrogen ratios, such as sludge digestion liquor, landfill leachate, or special industrial wastewaters. CANR can be achieved with two reactors in series: i) the SHARON reactor, which stands for Single reactor High activity Ammonia Removal Over Nitrite, (Hellinga et al. 1998), where the partial nitrification of the ammonium by aerobic oxidizing bacteria (AOB) and ii) the Anammox (Anaerobic Ammonium Oxidation (Mulder et al. 1995)). This process presents some additional advantages, like the lowering of gases with greenhouse effect (CO2 and NO2) or the elimination of external carbon sources. Its main drawback is related to the low growth rate of Anammox bacteria, involving the use of sludge retention systems, e.g. membranes, granular systems. Besides, in order to achieve a high elimination of all the nitrogen sources, it must be ensured that the ammonium and nitrite are fed in stable, close to equimolar proportions to the Anammox section. Therefore, a performing control system is essential to ensure the balance between ammonium and nitrite to the Anammox reactor. Some strategies have been applied in this field in order to optimize the nitrogen removal costs (Volcke et al. 2005) based in different control loops for the key variables in the process, as pH or dissolved oxygen (DO). The goal of this contribution is to present a stepwise assessment and design of a control system for the SHARON-Anammox process in two reactor configuration. The design focuses on two characteristics common to other wastewater treatment units: the scarcity of degrees of freedom/actuators and the high frequency of disturbances coming from upstream processes and/or inflow variations. Thus, the controlled variables are first screened by their ability to reject disturbances in order to build the regulatory layer. Then, some loops are cascaded in order to address the objectives of the system and improve its performance.

This contribution is organized as follows: first the reactors and their models are quickly presented, including the method for pH calculation. Secondly, the operating point and degrees of freedom are defined. Then, the effect of disturbances is assessed, giving place to the possible control structures. Finally, the designed structures are compared by evaluation with a simulated influent.

2. METHODS

2.1 Reactor description

The case study used in this work is adapted from an experimental description previously reported (Galí et al. 2007). The SHARON reactor is a continuous stirred tank reactor (CSTR) with a volume of 4 L and a hydraulic retention time of 1 day, with operating conditions 35°C, pH 7.23 and dissolved oxygen 1.06 g m^{-3} (the determination of optimal pH and DO is done in section 3.1), which implies an nominal kla of 192 d^{-1} at steady state conditions. The influent composition is 700 N- g m^{-3} of ammonium, 600 C- g m^{-3} of bicarbonate (equimolar) and 27 g m^{-3} of inorganic phosphorous. The Anammox reactor is modeled as a 20 L CSTR with a membrane as retention system that allows the growth of the bacteria. The temperature in this reactor is 30°C and the pH 7.95. The oxygen concentration corresponds to the residual oxygen coming from the upstream SHARON reactor.

2.2 Reactor modeling

The model used to describe the process is adapted from previously published work by Hellinga et al. (Hellinga, Van Loosdrecht & Heijnen 1999) and Volcke (Volcke 2006). The compartment was modeled as a CSTR. Assuming that the reactor hold-up and all the inflows and outflows have the same constant density, the total and partial mass balances are:

$$\frac{dV}{dt} = \sum_{i=1}^{n} F_i^{IN} - F^{OUT} \quad (1)$$

$$\frac{d(V \cdot C_i)}{dt} = F_i^{IN} \cdot C_i^{IN} - F^{OUT} \cdot C_i + k_L a \cdot (C_i^* - C_i) \cdot V + r_i \cdot V \quad (2)$$

where F stands for the volumetric flows, C for the concentrations, r for the reaction rate and V for the volume of the reactor. The subscripts $_{IN}$ and $_{OUT}$ stand for inflow and outflow respectively, $_i$ for each component and * for the equilibrium concentrations. The individual mass balances developed are described for the lumped compounds, i.e. ionized and unionized forms. The components considered are: H^+, NH_4^+, NH_3, HNO_2, NO_2^-, CO_2, HCO_{3-}, CO_3^{2-}, $H_2PO_4^-$, HPO_4^{2-}, NO_3^-, O_2, N_2, ammonia oxidizing bacteria (AOB), nitrite oxidizing bacteria (NOB), heterotrophic bacteria (HB) and Z (charge not involved in biological reactions). Absorption or stripping in (2) only applies for O_2 and CO_2. The partition coefficients of O_2 and CO_2 are determined by Henry's law (Villadsen, Nielsen & Liden 2011).

2.3 Reaction modeling

Five different biological reactions are included in the SHARON model. The nitrification process is divided in two different steps: the oxidation of the ammonia to nitrite, carrying out by AOB, and the oxidation of the nitrite to nitrate, carrying out by NOB. In order to take account of the microbial growth in the mass balances, the biomass composition is fixed as $CH_{1.8}O_{0.5}N_{0.2}$. The stoichiometric matrix and the expressions of the process rates for the two reactors have been taken from the literature.(Vangsgaard et al. 2012).

2.4 Determination of pH

The microbial activity affects to the pH since the reactions imply a production (partial nitrification) of protons. The pH is determined solving the corresponding mass balances (3a-d), equilibrium equations (4a-f) and charge balance (5). The resulting system of 13 nonlinear equations is solved by a multidimensional Newton-Raphson method adapted from Luff et al. (Luff, Haeckel & Wallmann 2001).

$$0 = TNH - (NH_4^+ + NH_3) \quad (3a)$$
$$0 = TNO - (HNO_2 + NO_2^-) \quad (3b)$$
$$0 = TIC - (CO_2 + HCO_3^- + CO_3^-) \quad (3c)$$
$$0 = TIP - (H_2PO_4^- + HPO_4^{2-}) \quad (3d)$$
$$0 = K_w - OH^- \cdot H^+ \quad (4a)$$
$$0 = K_{e,NH4} \cdot NH_4^+ - NH_3 \cdot H^+ \quad (4b)$$
$$0 = K_{e,HNO2} \cdot HNO_2 - NO_2^- \cdot H^+ \quad (4c)$$
$$0 = K_{e,CO2} \cdot CO_2 - HCO_3^- \cdot H^+ \quad (4d)$$
$$0 = K_{e,HCO3} \cdot HCO_3^- - CO_3^{2-} \cdot H^+ \quad (4e)$$
$$0 = K_{e,H2PO4} \cdot H_2PO_4^- - HPO_4^{2-} \cdot H^+ \quad (4f)$$
$$0 = Z^+ - NO_3^- - HCO_3^- - 2 \cdot CO_3^{2-} - H_2PO_4^- - 2HPO_4^{2-} NO_2^- - OH^- + NH_4^+ + H^+ \quad (5)$$

2.5 Controller modelling

All the controllers used in this work are proportional-integral controllers (PI). Sensors and actuators are modeled as perfect (immediate response with perfect accuracy) given the slow response of the system. Unless stated otherwise, the controllers were tuned using the internal model control guidelines (Seborg, Edgar & Mellichamp 2004).
The model was implemented and solved in Simulink environment in MATLAB R2009b (The MathWorks, Natick, MA).

3. CONTROL STRUCTURE DESIGN

3.1 Determination of operating conditions

As a previous step to control design, the optimal operation conditions in the SHARON reactor were determined mapping the effect of pH and dissolved oxygen (DO) in the performance of the reactor. The bounds considered were between 6.5 and 8 for pH, and between 0 g m^{-3} and 8.96 g m^{-3} (saturation, not shown in the figure) for DO. For each value of oxygen and pH the steady state was determined and, in particular, the ratio between the total number of nitrite moles (i.e. nitrous acid plus the nitrite anion, TNO) and the total number of ammonium moles (i.e. the ammonium cation plus ammonia, TNH) was recorded. The optimal TNO_2/TNH ratio in the influent of an Anammox reactor is 1.3 provided that anaerobic oxidation is the only reaction taking place (Van de Graaf et al. 1995). The dependency of the TNO_2/TNH ratio shows a maximum at pH 7.23 and a monotonous increase with DO which stabilizes asymptotically for excess of oxygen (Fig. 1). Therefore, in order to operate at minimum DO, and as a consequence decrease the needs of aeration, the operating conditions were selected as pH=7.23 and DO=1.06 g m^{-3}, corresponding to a ratio TNO_2/TNH of 1.3.

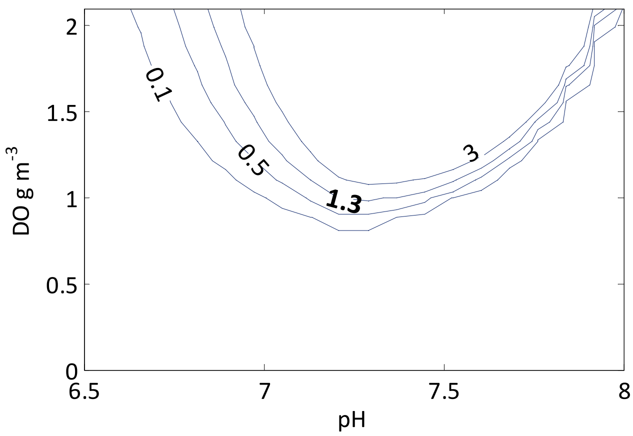

Fig. 1. Contour plot of the molar ratio TNO_2/TNH in function of pH and DO levels at steady state

3.2 Control objectives and degrees of freedom analysis

As stated earlier, the goal of the SHARON reactor is to provide a stable feed for the Anammox reactor of with a molar ratio TNO_2/TNH of 1.3. This is the primary objective that can be achieved using the molar ratio TNO_2/TNH as a control variable or can be approximated by keeping the system at the selected operating conditions. If the SHARON reactor is directly fed from a digester, the feed flow is a disturbance and therefore the level has to be controlled using the outflow as a manipulated variable (MV). As a consequence, there are only two manipulated variables left: aeration (represented by k_La) and the acid/base flow. The identified controlled variables (CV) and disturbances are summarized in Fig. 2.

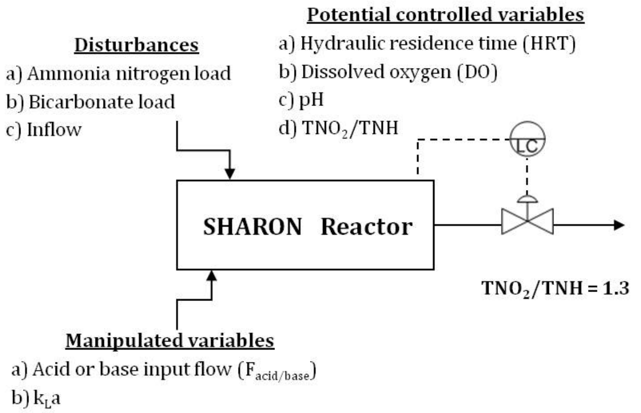

Fig. 2. Diagram of the SHARON reactor displaying the manipulated variables, the disturbances and candidates to controlled variables.

3.3 Assessment of disturbance effect and pairing

One of the main difficulties in the control of the SHARON reactor is the limited number of available actuators. Indeed, the four CV cannot be controlled simultaneously. The hydraulic residence time (HRT) must be kept above 0.89 days in order to ensure that the AOB are not washed out at the operating conditions. We decided to keep it uncontrolled but at a nominal value of 1 day to ensure that the disturbances in the feed flow would not decrease it below the limit of 0.89 days. Out of the three remaining CV, it can be argued that the most important is the ratio TNO_2/TNH since it is the primary objective of the system, although pH and DO are essential to keep the reactor stable. In order to rationally screen the CV to be paired with the available MVs, we assessed the pairings that would reject most easily the disturbances at different frequencies by the closed loop disturbance gain (CLDG) (Hovd, Skogestad 1992).

The CLDG is defined as:

$$CLDG \equiv \Delta = diag(G)G^{-1}G_d \qquad (6)$$

where G is the plant transfer function, diag(G) is the matrix consisting of diagonal elements of G and G_d is the disturbance transfer function. Both transfer functions were obtained with the linearization tool available in Simulink. The magnitude of the CLDG element δ_{ij} indicates the effect of the ith disturbance on the jth controlled variable at any given frequency. If the variables are suitably scaled, a δ_{ij} lower than 1 indicates that the disturbance will not lead the controlled variable to an unacceptable offset. The manipulated variables were scaled around their nominal values and the disturbances around ±10% of their nominal values. The controlled variables were scaled the following way: the maximum offset considered for the ratio TNO_2/TNH was ±0.5. Then, the equivalent deviation in DO and pH was determined with the data from Fig. 1, resulting in 0.16 g m^{-3} for DO and 0.2 units for pH.

The CLDG plots were obtained for the three combinations of CV-MV and the three disturbances (Fig. 3 and 4). The CLDG plots for the bicarbonate load are not shown since all the elements were well below 1.

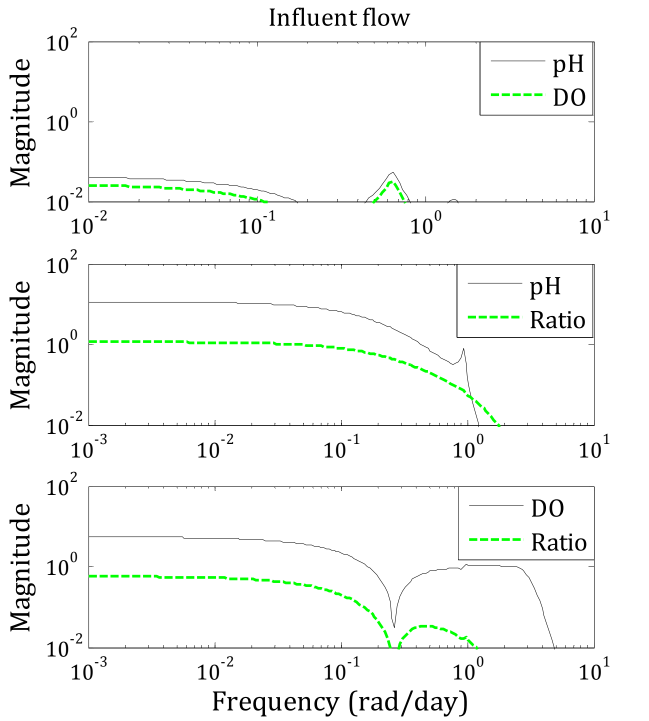

Fig. 3. CLDG plots for a disturbance in the influent flow

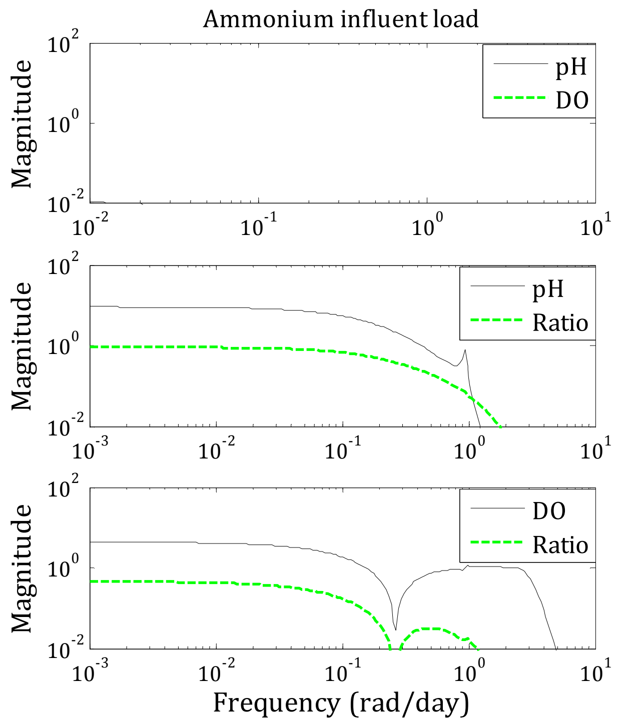

Fig. 4. CLDG plots for a disturbance in the ammonium influent load. Note that the elements in the top figure are lower than 10^{-2}

From the CLDG plots it is clear that the structure that pairs the MV with the pH and the DO have CLDG elements with lower magnitude at all the frequencies. Hence, this structure manages to rejects the disturbances more efficiently than those which consider the TNO_2/TNH ratio directly as a CV. Therefore the decentralized control structure used to stabilize the system is $F_{acid/base}$ – pH and k_La – DO. However, this structure cannot ensure that the TNO_2/TNH ratio will be kept at its optimal value. Therefore, a second structure is proposed where the setpoint for DO is set by a master loop controlling the TNO_2/TNH ratio (Fig. 5).

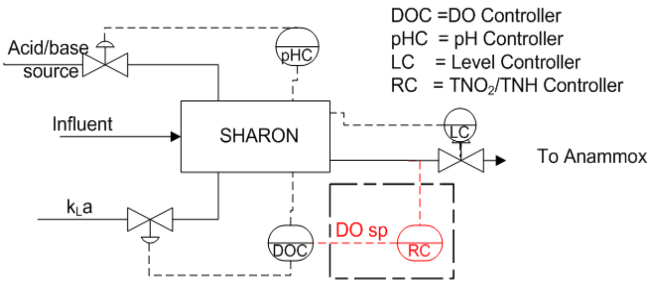

Fig. 5. Control structures for SHARON reactor. The master loop inside the dashed box is only active in the second control structure.

3.4 Regulation and feedback from the Anammox reactor

The proposed control structures deal with regulation of the SHARON reactor and, in the case of the cascaded structure, with control of the TNO_2/TNH ratio. Since the Anammox reactor is run at anoxic conditions, only one actuator can be used upon it: the addition of sodium bicarbonate to regulate the pH. This strategy can effectively regulate the reactor operation but fails to address the control objective of maximizing nitrogen removal. In principle, if the TNO_2/TNH ratio in the feed to the Anammox reactor is kept at the optimum value, the removal of nitrogen is maximized. However, this design ratio may vary in the dynamic operation for a number of reasons: entrainment of AOB to the Anammox reactor that keep oxidizing ammonium and hence changing the relative amounts of nitrogen compounds, model mismatch due to microorganism evolution, presence of heterotroph bacteria... In order to tackle those factors, a nested cascaded structure is proposed (fig. 6) where a master loop modifies the TNO_2/TNH ratio setpoint according to the concentration of nitrite in the Anammox reactor. This structure provides feedback upstream improving the performance of the whole process. It must be borne in mind that the AnAOB bacteria, present in the second reactor, have a considerably slow growth rate. Hence, it is more convenient to reduce the disturbances upstream, before they upset the operation of the Anammox reactor. The nested cascade structure is indeed more complex than the others but the loops work at a very different frequency range, giving place to the needed time-scale separation for a suitable operation.

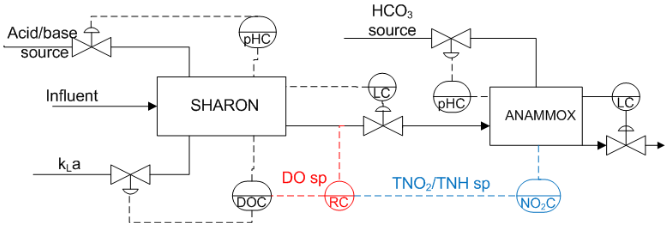

Fig. 6. Three proposed control structures: regulatory (black), cascaded (red), and nested cascade (blue).

5. RESULTS

The three proposed control structures were tested for disturbance rejection using a simulated influent used for benchmarking. The selected influent is the benchmark simulating model 2 (BSM2, (Nopens et al. 2010)) outflow of the anaerobic digester for 30 days (fig. 7). Only the last 15 days are considered for evaluation. The influent features a number of state variables, among them soluble inert organic matter, readily biodegradable substrate, particulate inert organic matter, slowly biodegradable substrate, active heterotrophic biomass, total ammonium nitrogen, soluble biodegradable organic nitrogen, particulate biodegradable organic nitrogen, alkalinity, total suspended solids, temperature and total flowrate. The influent also considers variations in temperature and takes into account diurnal and weekly variations in flow rate and rainfall.

Two types of performance indicators were determined: the integral of absolute error, which measures the offset of the controlled variables and the total variance of manipulated variables, which represents the variations in control action needed to reject the disturbance.

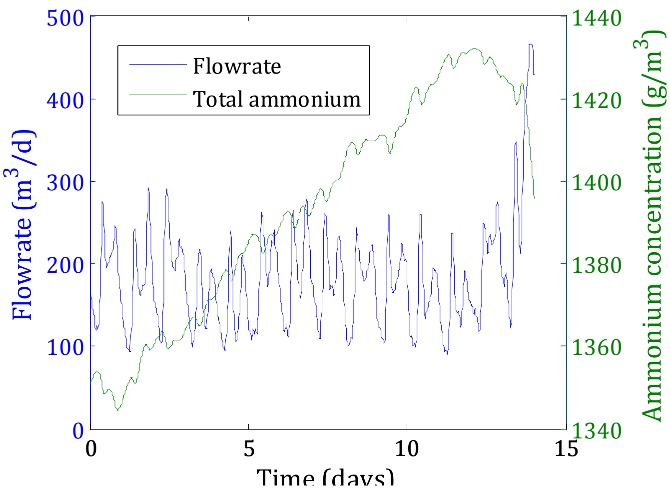

Fig.7 Incoming flowrate and ammonium concentration in the influent to the process corresponding to the fall season. Note the peak after 13 days due to a rain event.

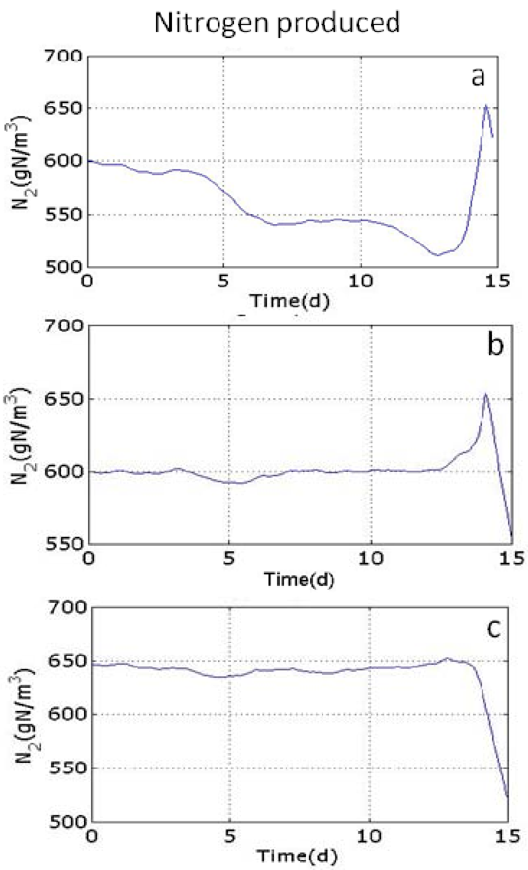

Fig. 8. Production of nitrogen gas in the Anammox reactor for 15 days of evaluation with the BSM2 anaerobic digester effluent: a) regulatory structure, b) cascade, c) nested cascade

The results of the simulation show that the addition of the first cascaded loop improves the regulation of the process making the production of nitrogen (and thereby the nitrogen removal) robust to the influent disturbances. The addition of the second cascade does not have a major impact on the regulation of the process but it leads to a maximization of the nitrogen removal from the system allowing to improve the percentage of nitrogen removed in 6% of the total initial (table 1). Besides, the addition of the cascaded structures did not increase the regulation effort in the other loops as the total variation of the pH loop actuator in the SHARON reactor decreased considerably.

As a conclusion, the three structures were suitable to regulate the system but the performance in nitrogen removal was improved by increasing the complexity through cascaded loops that act as supervisory controllers. Given the position of the nitrogen removal process in a wastewater treatment plant, the three structures can be suitable depending on the requirements of the downstream treatment. For example, high nitrogen removal may be needed for highly loaded water (e.g. pig manure) but a moderate removal may be sufficient if a conventional denitrification treatment is placed downstream.

Table 1. Key performance indicators for the control structures proposed for 15 days of evaluation with the BSM2 anaerobic digester effluent. Note that the IAE of DO is very high in the cascaded controllers due to the sudden setpoint change.

Structure	**Nitrogen removal**		**DO loop**	**pH loop**
Regulatory	**78.1%**	IAE	0.45 d	1.79 d
		TV	336 d^{-1}	$2.25\cdot10^{-4}$ m^3d^{-1}
Cascade	**85.7%**	IAE	1.12 d	1.96 d
		TV	$4.95\cdot10^3$ d^{-1}	$5.90\cdot10^{-5}$ m^3 d^{-1}
Nested cascade	**91.4%**	IAE	1.68 d	1.83 d
		TV	$3.73\cdot10^3$ d^{-1}	$5.30\cdot10^{-5}$ m^3 d^{-1}

6. CONCLUSIONS

The pH and DO concentration for SHARON were determined for and optimal TNO_2/TNH ratio of 1.3 in order to feed a downstream Anammox reactor. The operating conditions found were pH 7.23 and DO 1.06 g m^{-3}. For the optimised steady state, we used the closed loop disturbance gain (CLDG) as a measurement of the effect of disturbances in the reactor. Hence, three control structures were proposed for the SHARON-Anamox process, as a first stage in autotrophic nitrogen removal. The performance, evaluated with a simulated influent, confirmed the CLDG results and, therefore, a cascaded decentralized structure is proposed as a suitable configuration to maximise nitrogen removal. Special attention was given to the scarcity of actuators in the process.

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